

Cyclophosphamide
50-18-0 | DTXSID5020364

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 73.0 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.09e-01

Confidence level: 6.03e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Uracil mustard</div> <div>Measured: 28.8</div> <div>Predicted: 37.5</div>	<div>Image not found</div> <div>Oxamyl</div> <div>Measured: 10.0</div> <div>Predicted: 15.0</div>	<div>Image not found</div> <div>Trietazine</div> <div>Measured: 575</div> <div>Predicted: 407</div>
<div>Image not found</div> <div>Methabenzthiazuron</div> <div>Measured: 631</div> <div>Predicted: 107</div>	<div>Image not found</div> <div>Bromacil</div> <div>Measured: 39.8</div> <div>Predicted: 51.5</div>	